

# Best Linear Unbiased Prediction (BLUP)

## Best Linear Unbiased Prediction (BLUP):

Suppose

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where

$$E(\boldsymbol{\varepsilon}) = \mathbf{0}, \quad \text{and} \quad \text{Var}(\boldsymbol{\varepsilon}) = \boldsymbol{\Sigma} = \sigma^2\mathbf{V}.$$

Initially, we will assume the Aitken model holds so that  $\sigma^2 > 0$  is unknown and  $V$  is a known symmetric and PD matrix.

Suppose  $u$  is a random variable with mean 0 and finite variance.

A linear predictor  $d + \mathbf{a}'\mathbf{y}$  of  $\mathbf{c}'\boldsymbol{\beta} + u$  is unbiased iff

$$E(d + \mathbf{a}'\mathbf{y}) = E(\mathbf{c}'\boldsymbol{\beta} + u) = \mathbf{c}'\boldsymbol{\beta} \quad \forall \boldsymbol{\beta} \in \mathbb{R}^p.$$

$c'\beta + u$  is predictable iff  $\exists$  an unbiased linear predictor of  $c'\beta + u$ .

Note that  $\mathbf{c}'\boldsymbol{\beta} + u$  is predictable  $\iff \exists \mathbf{a} \ni \mathbf{c}' = \mathbf{a}'\mathbf{X}$ .

This follows from the same argument used to show that  $\mathbf{c}'\boldsymbol{\beta}$  estimable  $\iff \exists \mathbf{a} \ni \mathbf{c}' = \mathbf{a}'\mathbf{X}$ .

Also,  $d + \mathbf{a}'\mathbf{y}$  is an unbiased predictor of  $\mathbf{c}'\boldsymbol{\beta} + u$  iff

$$d = 0 \quad \text{and} \quad \mathbf{c}' = \mathbf{a}'\mathbf{X},$$

as argued for the case of an unbiased estimator.

Suppose  $\hat{w}$  is a predictor of a random variable  $w$ .

The mean squared error (MSE) of  $\hat{w}$  as a predictor of  $w$  is

$$E(\hat{w} - w)^2.$$



Suppose

$$\text{Cov}(\boldsymbol{\varepsilon}, u) = \sigma^2 \mathbf{k}$$

for some known vector  $\mathbf{k}$ .

Suppose  $\mathbf{c}'\boldsymbol{\beta} + u$  is predictable.

Prove that  $\mathbf{c}'\hat{\boldsymbol{\beta}}_{\text{GLS}} + \hat{u}$  has lowest MSE among all unbiased linear predictors of  $\mathbf{c}'\boldsymbol{\beta} + u$ , where

$$\hat{u} \equiv [\text{Cov}(\boldsymbol{\varepsilon}, u)]' [\text{Var}(\boldsymbol{\varepsilon})]^{-1} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{\text{GLS}}) = \mathbf{k}' \mathbf{V}^{-1} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{\text{GLS}}).$$

## Proof:

First note that

$$\mathbf{c}'\hat{\boldsymbol{\beta}}_{\text{GLS}} + \hat{u} = \mathbf{c}'\hat{\boldsymbol{\beta}}_{\text{GLS}} + \mathbf{k}'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{\text{GLS}})$$

has expectation

$$\mathbf{c}'\boldsymbol{\beta} + \mathbf{k}'\mathbf{V}^{-1}(\mathbf{X}\boldsymbol{\beta} - \mathbf{X}\boldsymbol{\beta}) = \mathbf{c}'\boldsymbol{\beta}.$$

Thus,  $\mathbf{c}'\hat{\boldsymbol{\beta}}_{\text{GLS}} + \hat{u}$  is an unbiased predictor of  $\mathbf{c}'\boldsymbol{\beta} + u$ .

Now note that

$$\begin{aligned} \mathbf{c}'\hat{\boldsymbol{\beta}}_{\text{GLS}} + \hat{u} &= \mathbf{c}'\hat{\boldsymbol{\beta}}_{\text{GLS}} + \mathbf{k}'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{\text{GLS}}) \\ &= (\mathbf{c}' - \mathbf{k}'\mathbf{V}^{-1}\mathbf{X})\hat{\boldsymbol{\beta}}_{\text{GLS}} + \mathbf{k}'\mathbf{V}^{-1}\mathbf{y} \\ &= (\mathbf{c}' - \mathbf{k}'\mathbf{V}^{-1}\mathbf{X})(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y} + \mathbf{k}'\mathbf{V}^{-1}\mathbf{y} \\ &= [(\mathbf{c}' - \mathbf{k}'\mathbf{V}^{-1}\mathbf{X})(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1} + \mathbf{k}'\mathbf{V}^{-1}]\mathbf{y} \\ &\equiv \mathbf{b}'\mathbf{y} \quad (\text{a linear estimator.}) \end{aligned}$$

Because

$$\mathbf{c}'\hat{\boldsymbol{\beta}}_{\text{GLS}} + \hat{u} = \mathbf{b}'\mathbf{y}$$

is an unbiased predictor, we know

$$\mathbf{b}'\mathbf{X} = \mathbf{c}'.$$

Let  $a'y$  be any other linear unbiased predictor of  $c'\beta + u$ . Then  $a'X = c'$ .

The MSE of  $\mathbf{a}'\mathbf{y}$  is

$$\begin{aligned} E[\mathbf{a}'\mathbf{y} - (\mathbf{c}'\boldsymbol{\beta} + u)]^2 &= \text{Var}[\mathbf{a}'\mathbf{y} - (\mathbf{c}'\boldsymbol{\beta} + u)] \\ &= \text{Var}(\mathbf{a}'\mathbf{y} - u) \\ &= \text{Var}(\mathbf{a}'\mathbf{y} - \mathbf{b}'\mathbf{y} - u + \mathbf{b}'\mathbf{y}) \\ &= \text{Var}[(\mathbf{a} - \mathbf{b})'\mathbf{y}] + \text{Var}(\mathbf{b}'\mathbf{y} - u) \\ &\quad + 2\text{Cov}[(\mathbf{a} - \mathbf{b})'\mathbf{y}, \mathbf{b}'\mathbf{y} - u]. \end{aligned}$$

Now

$$\begin{aligned}\text{Cov}[(\mathbf{a} - \mathbf{b})'\mathbf{y}, \mathbf{b}'\mathbf{y} - u] &= (\mathbf{a} - \mathbf{b})'\text{Var}(\mathbf{y})\mathbf{b} - \text{Cov}[(\mathbf{a} - \mathbf{b})'\mathbf{y}, u] \\ &= (\mathbf{a} - \mathbf{b})'\sigma^2\mathbf{V}\mathbf{b} - (\mathbf{a} - \mathbf{b})'\text{Cov}(\mathbf{y}, u) \\ &= \sigma^2(\mathbf{a} - \mathbf{b})'\mathbf{V}\mathbf{b} - (\mathbf{a} - \mathbf{b})'\text{Cov}(\boldsymbol{\varepsilon}, u) \\ &= \sigma^2(\mathbf{a} - \mathbf{b})'\mathbf{V}\mathbf{b} - \sigma^2(\mathbf{a} - \mathbf{b})'\mathbf{k} \\ &= \sigma^2(\mathbf{a} - \mathbf{b})'(\mathbf{V}\mathbf{b} - \mathbf{k}).\end{aligned}$$

Now

$$\begin{aligned}Vb - k &= V[V^{-1}X[(X'V^{-1}X)^{-1}]'(c - X'V^{-1}k) + V^{-1}k] - k \\ &= X[(X'V^{-1}X)^{-1}]'(c - X'V^{-1}k).\end{aligned}$$

Thus, the covariance term is

$$\sigma^2(\mathbf{a} - \mathbf{b})'X[(X'V^{-1}X)^{-1}]'(c - X'V^{-1}k),$$

which is 0 because

$$\mathbf{a}'X = \mathbf{b}'X = \mathbf{c}'.$$



Thus, we have

$$\begin{aligned}\text{MSE}(\mathbf{a}'\mathbf{y}) &= \text{Var}[(\mathbf{a} - \mathbf{b})'\mathbf{y}] + \text{Var}(\mathbf{b}'\mathbf{y} - u) \\ &= \text{Var}[(\mathbf{a} - \mathbf{b})'\mathbf{y}] + \text{Var}[\mathbf{b}'\mathbf{y} - (\mathbf{c}'\boldsymbol{\beta} + u)] \\ &= \text{Var}[(\mathbf{a} - \mathbf{b})'\mathbf{y}] + E[\mathbf{b}'\mathbf{y} - (\mathbf{c}'\boldsymbol{\beta} + u)]^2 \\ &= \text{Var}[(\mathbf{a} - \mathbf{b})'\mathbf{y}] + \text{MSE}(\mathbf{b}'\mathbf{y}).\end{aligned}$$

Thus,

$$\text{MSE}(\mathbf{a}'\mathbf{y}) \geq \text{MSE}(\mathbf{b}'\mathbf{y})$$

with equality iff

$$\text{Var}[(\mathbf{a} - \mathbf{b})'\mathbf{y}] = 0 \iff \mathbf{a} = \mathbf{b}.$$

Thus  $\mathbf{c}'\hat{\boldsymbol{\beta}}_{\text{GLS}} + \hat{u}$  is the unique best linear unbiased predictor (BLUP) of  $\mathbf{c}'\boldsymbol{\beta} + u$ . □

In practice,

$$\Sigma = \sigma^2 \mathbf{V}$$

involves unknown variance components in addition to the unknown  $\sigma^2$ .

We replace unknown variance components in  $c' \hat{\beta}_{GLS} + \hat{u}$  by the estimates to obtain “empirical” BLUPs (eBLUPs).

This typically results in a nonlinear predictor whose properties are not so well characterized.

## Example:

Suppose  $y_{ij}$  is the average monthly milk production of the  $j^{\text{th}}$  daughter of sire  $i$ .

Suppose

$$y_{ij} = \mu + s_i + e_{ij} \quad \text{for } i = 1, \dots, t; j = 1, \dots, n_i,$$

where  $s_1, \dots, s_t$  are iid with mean 0 and variance  $\sigma_s^2$ ,

independent of the  $e_{ij}$  terms, which are iid with mean 0 and variance  $\sigma_e^2$ .

Suppose  $\sigma_s^2/\sigma_e^2$  is a known constant  $d$ .

Find an expression for the BLUP of  $\mu + s_1$ .

Let  $\mathbf{y} = [y_{11}, \dots, y_{1n_1}, y_{21}, \dots, y_{2n_2}, \dots, y_{m_t}]'$ .

Let  $\mathbf{X} = \mathbf{1}_{n \times 1}$  where  $n = \sum_{i=1}^t n_i$ .

Let  $\boldsymbol{\beta} = [\mu]$ .

Let  $\boldsymbol{\varepsilon} = \begin{bmatrix} s_1 + e_{11} \\ \vdots \\ s_1 + e_{1n_1} \\ s_2 + e_{21} \\ \vdots \\ s_2 + e_{2n_2} \\ \vdots \\ s_t + e_{tn_t} \end{bmatrix}$ .

Then  $\text{Var}(\boldsymbol{\varepsilon})$  is block diagonal with blocks of sizes

$n_1 \times n_1, n_2 \times n_2, \dots, n_t \times n_t$ .

Each block has  $\sigma_s^2 + \sigma_e^2$  on the diagonal and  $\sigma_s^2$  on the off-diagonal.

The  $i^{\text{th}}$  block is

$$\sigma_e^2 \mathbf{I}_{n_i \times n_i} + \sigma_s^2 \mathbf{1}\mathbf{1}' = \sigma_e^2 [\mathbf{I} + d\mathbf{1}\mathbf{1}'].$$



We wish to predict  $\mathbf{c}'\boldsymbol{\beta} + u$ , where  $\mathbf{c} = [1]$ ,  $\boldsymbol{\beta} = [\mu]$  and  $u = s_1$ .

$$\begin{aligned}\text{Cov}(\boldsymbol{\varepsilon}, u) &= \text{Cov}(\boldsymbol{\varepsilon}, s_1) = \begin{bmatrix} \sigma_s^2 \mathbf{1}_{n_1 \times 1} \\ \mathbf{0}_{(n-n_1) \times 1} \end{bmatrix} \\ &= \sigma_e^2 \begin{bmatrix} d \mathbf{1}_{n_1 \times 1} \\ \mathbf{0}_{(n-n_1) \times 1} \end{bmatrix} \equiv \sigma_e^2 \mathbf{k}.\end{aligned}$$

We need  $\hat{\beta}_{\text{GLS}}$ , a solution to the Aitken equations

$$\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{V}^{-1}\mathbf{y},$$

where

$$\mathbf{V} = \text{diag}\left(\begin{matrix} \mathbf{I} & \\ & d\mathbf{1}\mathbf{1}' \end{matrix}_{n_1 \times n_1}, \dots, \begin{matrix} \mathbf{I} & \\ & d\mathbf{1}\mathbf{1}' \end{matrix}_{n_t \times n_t}\right).$$

$$\left(\begin{matrix} \mathbf{I} & \\ & d\mathbf{1}\mathbf{1}' \end{matrix}_{n_i \times n_i}\right)^{-1} = \begin{matrix} \mathbf{I} & \\ & \frac{d}{1 + dn_i} \mathbf{1}\mathbf{1}' \end{matrix}_{n_i \times n_i}.$$

Thus,

$$\begin{aligned} X'V^{-1}X &= \mathbf{1}'V^{-1}\mathbf{1} \\ &= \sum_{i=1}^t \mathbf{1}' \left[ \mathbf{I} - \frac{d}{1 + dn_i} \mathbf{1}\mathbf{1}' \right] \mathbf{1} \\ &= \sum_{i=1}^t \left( n_i - \frac{dn_i^2}{1 + dn_i} \right) \\ &= \sum_{i=1}^t \frac{n_i}{1 + dn_i}. \end{aligned}$$

$$\begin{aligned}
\mathbf{X}'\mathbf{V}^{-1}\mathbf{y} &= \sum_{i=1}^t \mathbf{1}' \left[ \mathbf{I} - \frac{d}{1 + dn_i} \mathbf{1}\mathbf{1}' \right] \mathbf{y}_i \\
&\quad (\text{where } \mathbf{y}_i = [y_{i1}, \dots, y_{in_i}]') \\
&= \sum_{i=1}^t \left( y_{i\cdot} - \frac{dn_i}{1 + dn_i} y_{i\cdot} \right) \\
&= \sum_{i=1}^t \left( 1 - \frac{dn_i}{1 + dn_i} \right) y_{i\cdot} \\
&= \sum_{i=1}^t \frac{n_i}{1 + dn_i} \bar{y}_{i\cdot}
\end{aligned}$$

Thus,

$$\begin{aligned}\hat{\beta}_{\text{GLS}} &= \hat{\mu}_{\text{GLS}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y} \\ &= \frac{\sum_{i=1}^t \frac{n_i}{1+dn_i} \bar{y}_i}{\sum_{i=1}^t \frac{n_i}{1+dn_i}} \\ &= \frac{\sum_{i=1}^t (\sigma_e^2/n_i + \sigma_s^2)^{-1} \bar{y}_i}{\sum_{i=1}^t (\sigma_e^2/n_i + \sigma_s^2)^{-1}}.\end{aligned}$$

Note that each  $\bar{y}_i$  is an unbiased estimator of  $\mu$  with variance

$$\sigma_e^2/n_i + \sigma_s^2.$$

Thus,  $\hat{\mu}_{\text{GLS}}$  is a weighted average of independent unbiased estimators of  $\mu$ , with inverse variances of estimators as weights.

Now,

$$\hat{s}_1 = \hat{u} = \mathbf{k}'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\hat{\beta}_{\text{GLS}})$$

$$\begin{aligned} \mathbf{k}'\mathbf{V}^{-1}\mathbf{y} &= d\mathbf{1}' \left[ \mathbf{I} - \frac{d}{1 + dn_1} \mathbf{1}\mathbf{1}' \right] \mathbf{y}_1 \\ &= dy_{1\cdot} - \frac{d^2 n_1}{1 + dn_1} y_{1\cdot} \\ &= \frac{d + d^2 n_1 - d^2 n_1}{1 + dn_1} y_{1\cdot} \\ &= \frac{dn_1}{1 + dn_1} \bar{y}_{1\cdot\cdot} \end{aligned}$$

$$\begin{aligned} \mathbf{k}'\mathbf{V}^{-1}\mathbf{X}\hat{\boldsymbol{\beta}}_{\text{GLS}} &= d\mathbf{1}'\left[\mathbf{I} - \frac{d}{1+dn_1}\mathbf{1}\mathbf{1}'\right]\mathbf{1}\hat{\mu}_{\text{GLS}} \\ &= \left(dn_1 - \frac{d^2n_1^2}{1+dn_1}\right)\hat{\mu}_{\text{GLS}} \\ &= \frac{dn_1}{1+dn_1}\hat{\mu}_{\text{GLS}}. \end{aligned}$$



Thus, the BLUP of  $\mu + s_1$  is

$$\begin{aligned} & \hat{\mu}_{\text{GLS}} + \frac{dn_1}{1 + dn_1} \bar{y}_{1\cdot} - \frac{dn_1}{1 + dn_1} \hat{\mu}_{\text{GLS}} \\ &= \frac{dn_1}{1 + dn_1} \bar{y}_{1\cdot} + \left( 1 - \frac{dn_1}{1 + dn_1} \right) \hat{\mu}_{\text{GLS}} \\ &= \frac{\sigma_s^2}{\sigma_e^2/n_1 + \sigma_s^2} \bar{y}_{1\cdot} + \frac{\sigma_e^2/n_1}{\sigma_e^2/n_1 + \sigma_s^2} \hat{\mu}_{\text{GLS}}. \end{aligned}$$

The mean squared error (MSE) of a predictor  $\hat{\boldsymbol{w}}$  of a random vector  $\boldsymbol{w}$  is

$$\text{MSE}(\hat{\boldsymbol{w}}) = E[(\hat{\boldsymbol{w}} - \boldsymbol{w})(\hat{\boldsymbol{w}} - \boldsymbol{w})'].$$

Now suppose  $\mathbf{u}$  is a random vector with mean  $\mathbf{0}$  and  
 $\text{Cov}(\boldsymbol{\varepsilon}, \mathbf{u}) = \sigma^2 \underset{n \times q}{\overset{q \times 1}{\mathbf{K}}}$ .

The BLUP of predictable  $\mathbf{C}\boldsymbol{\beta} + \mathbf{u}$  is  $\mathbf{C}\hat{\boldsymbol{\beta}}_{\text{GLS}} + \hat{\mathbf{u}}$ , where

$$\hat{\mathbf{u}} \equiv [\text{Cov}(\boldsymbol{\varepsilon}, \mathbf{u})]' [\text{Var}(\boldsymbol{\varepsilon})]^{-1} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{\text{GLS}}) = \mathbf{K}'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{\text{GLS}}).$$

$C\hat{\beta}_{\text{GLS}} + \hat{\mathbf{u}}$  is the “best” linear unbiased predictor in the sense that

$$\text{MSE}(\hat{\mathbf{w}}) - \text{MSE}(C\hat{\beta}_{\text{GLS}} + \hat{\mathbf{u}})$$

is nonnegative definite  $\forall \hat{\mathbf{w}}$ , a linear unbiased predictor of  $C\beta + \mathbf{u}$ .

As for the case of univariate prediction, we replace unknown variance components in  $C\hat{\beta}_{\text{GLS}} + \hat{u}$  by their estimates to obtain an eBLUP whenever necessary.

For example, suppose

$$y = X\beta + Zu + e, \quad \text{where}$$

$$E(\mathbf{u}) = \mathbf{0} \quad E(\mathbf{e}) = \mathbf{0}$$

$$\text{Var}(\mathbf{u}) = \mathbf{G} \quad \text{Var}(\mathbf{e}) = \mathbf{R}$$

$$\text{Cov}(\mathbf{u}, \mathbf{e}) = \mathbf{0}.$$

Then, with  $\boldsymbol{\varepsilon} = \mathbf{Z}\mathbf{u} + \mathbf{e}$ , we have

$$\text{Var}(\boldsymbol{\varepsilon}) = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}$$

and

$$\begin{aligned}\text{Cov}(\boldsymbol{\varepsilon}, \mathbf{u}) &= \text{Cov}(\mathbf{Z}\mathbf{u} + \mathbf{e}, \mathbf{u}) \\ &= \text{Cov}(\mathbf{Z}\mathbf{u}, \mathbf{u}) \\ &= \mathbf{Z}\text{Cov}(\mathbf{u}, \mathbf{u}) \\ &= \mathbf{Z}\text{Var}(\mathbf{u}) \\ &= \mathbf{Z}\mathbf{G}.\end{aligned}$$

It follows that the BLUP of  $u$  is

$$GZ'(ZGZ' + R)^{-1}(y - X\hat{\beta}_{GLS}).$$



Similarly, if  $D$  is a known  $m \times q$  matrix, the BLUP of  $Du$  is

$$DGZ'(ZGZ' + R)^{-1}(\mathbf{y} - X\hat{\beta}_{\text{GLS}}).$$

When  $G$  and  $R$  are unknown, we use the eBLUP

$$D\hat{G}Z'(Z\hat{G}Z' + \hat{R})^{-1}(\mathbf{y} - X\hat{\beta}_{\text{GLS}}).$$

Note that computing  $\hat{\beta}_{\text{GLS}}$  or computing the BLUP of  $Du$  requires inversion of the  $n \times n$  matrix  $ZGZ' + R$ .

This can be computationally expensive.

We often assume that

$$\mathbf{R} = \sigma_e^2 \mathbf{I},$$

but even then

$$\mathbf{ZGZ}' + \sigma_e^2 \mathbf{I}$$

is a  $n \times n$  matrix that may be difficult to invert.

Until further notice, assume

$$\mathbf{R} = \sigma_e^2 \mathbf{I}$$

for some unknown  $\sigma_e^2 > 0$ .

Define  $\mathbf{H} = \frac{1}{\sigma_e^2} \mathbf{G}$ . Then

$$\begin{aligned} \text{Var}(\mathbf{y}) &= \mathbf{ZGZ}' + \sigma_e^2 \mathbf{I} \\ &= \sigma_e^2 (\mathbf{ZHZ}' + \mathbf{I}) = \sigma_e^2 \mathbf{V} \\ &\text{where } \mathbf{V} = \mathbf{ZHZ}' + \mathbf{I}. \end{aligned}$$

C.R. Henderson introduced the Mixed Model Equations(MME)

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z} \end{bmatrix} \begin{bmatrix} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{y} \\ \mathbf{Z}'\mathbf{y} \end{bmatrix}.$$

Recall that the Aitken equations are

$$\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\tilde{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{V}^{-1}\mathbf{y},$$

which in our special case are equivalent to

$$\mathbf{X}'(\mathbf{Z}\mathbf{H}\mathbf{Z}' + \mathbf{I})^{-1}\mathbf{X}\tilde{\boldsymbol{\beta}} = \mathbf{X}'(\mathbf{Z}\mathbf{H}\mathbf{Z}' + \mathbf{I})^{-1}\mathbf{y}.$$

Henderson showed that

(1) The MME are consistent.

(2) If  $\begin{bmatrix} \tilde{\beta} \\ \tilde{u} \end{bmatrix}$  solve the MME, then  $\tilde{\beta}$  is a solution to the AE (equivalently,  $X\tilde{\beta} = X\hat{\beta}_{GLS}$ ) and  $\tilde{u}$  is the BLUP of  $u$ .

(3) Conversely, if  $\tilde{\beta}$  solves the AE, then the MME have a solution whose leading subvector is  $\tilde{\beta}$ .



A nice thing about this result is that we can find  $\hat{\beta}_{\text{GLS}}$  and the BLUP of  $\mathbf{u}$  (or  $D\mathbf{u}$ ) without inverting the  $n \times n$  matrix  $(\mathbf{ZGZ}' + \sigma_e^2\mathbf{I})$ .

$$\begin{bmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z} \end{bmatrix}$$

is  $(p + q) \times (p + q)$ . In some problems,  $p + q \ll n$ .

By (2), the BLUP of a predictable  $C\beta + Du$  is given by

$$C\tilde{\beta} + D\tilde{u}$$

where  $\begin{bmatrix} \tilde{\beta} \\ \tilde{u} \end{bmatrix}$  solves the MME.

To prove Henderson's results, we begin with the following lemma.

Lemma H1: Suppose  $A$  is a symmetric and positive definite matrix. Suppose  $W$  is any matrix with number of columns equal to number of rows of  $A$ . Then

$$AW'(I + WAW')^{-1} = (A^{-1} + W'W)^{-1}W'.$$

## Proof:

First show that

$$\mathbf{I} + \mathbf{WAW}' \quad \text{and} \quad \mathbf{A}^{-1} + \mathbf{W}'\mathbf{W}$$

are each nonsingular.

$$\begin{aligned}
\forall \mathbf{x} \neq \mathbf{0}, \mathbf{x}'(\mathbf{I} + \mathbf{WAW}')\mathbf{x} &= \mathbf{x}'\mathbf{x} + \mathbf{x}'\mathbf{WAW}'\mathbf{x} \\
&= \|\mathbf{x}\|^2 + \|\mathbf{A}^{1/2}\mathbf{W}'\mathbf{x}\|^2 \\
&\geq \|\mathbf{x}\|^2 > 0.
\end{aligned}$$

Thus,  $\mathbf{I} + \mathbf{WAW}'$  is PD and  $\therefore$  nonsingular.

$$\begin{aligned}
\forall \mathbf{x} \neq \mathbf{0}, \mathbf{x}'(\mathbf{A}^{-1} + \mathbf{W}'\mathbf{W})\mathbf{x} &= \mathbf{x}'\mathbf{A}^{-1}\mathbf{x} + \mathbf{x}'\mathbf{W}'\mathbf{W}\mathbf{x} \\
&= \mathbf{x}'\mathbf{A}^{-1}\mathbf{x} + \|\mathbf{W}\mathbf{x}\|^2 \\
&\geq \mathbf{x}'\mathbf{A}^{-1}\mathbf{x} > 0
\end{aligned}$$

$\therefore \mathbf{A}$  PD  $\implies \mathbf{A}^{-1}$  PD.  $\therefore \mathbf{A}^{-1} + \mathbf{W}'\mathbf{W}$  is nonsingular.

Now show that

$$(\mathbf{A}^{-1} + \mathbf{W}'\mathbf{W})\mathbf{A}\mathbf{W}' = \mathbf{W}'(\mathbf{I} + \mathbf{W}\mathbf{A}\mathbf{W}')$$

and then complete the proof.

$$\begin{aligned}(\mathbf{A}^{-1} + \mathbf{W}'\mathbf{W})\mathbf{A}\mathbf{W}' &= \mathbf{A}^{-1}\mathbf{A}\mathbf{W}' + \mathbf{W}'\mathbf{W}\mathbf{A}\mathbf{W}' \\ &= \mathbf{W}' + \mathbf{W}'\mathbf{W}\mathbf{A}\mathbf{W}' \\ &= \mathbf{W}'(\mathbf{I} + \mathbf{W}\mathbf{A}\mathbf{W}').\end{aligned}$$

Multiplying on the left by

$$(\mathbf{A}^{-1} + \mathbf{W}'\mathbf{W})^{-1}$$

gives

$$\mathbf{A}\mathbf{W}' = (\mathbf{A}^{-1} + \mathbf{W}'\mathbf{W})^{-1}\mathbf{W}'(\mathbf{I} + \mathbf{W}\mathbf{A}\mathbf{W}').$$

Multiplying on the right by  $(\mathbf{I} + \mathbf{W}\mathbf{A}\mathbf{W}')^{-1}$  gives the result. □



Now use Lemma H1 to prove Lemma H2:

$$\begin{aligned} \mathbf{V}^{-1} &= (\mathbf{I} + \mathbf{Z}\mathbf{H}\mathbf{Z}')^{-1} \\ &= \mathbf{I} - \mathbf{Z}(\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'. \end{aligned}$$

## Proof:

Applying the Lemma H1 with  $\mathbf{H} = \mathbf{A}$  and  $\mathbf{Z} = \mathbf{W}$  yields

$$(\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}' = \mathbf{HZ}'(\mathbf{I} + \mathbf{ZHZ}')^{-1}. \quad (*)$$

Thus,

$$\begin{aligned} & [\mathbf{I} - \mathbf{Z}(\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'](\mathbf{I} + \mathbf{ZHZ}') \\ &= [\mathbf{I} - \mathbf{ZHZ}'(\mathbf{I} + \mathbf{ZHZ}')^{-1}](\mathbf{I} + \mathbf{ZHZ}') \text{ by } (*) \\ &= \mathbf{I} + \mathbf{ZHZ}' - \mathbf{ZHZ}' = \mathbf{I}. \end{aligned}$$



Now let's prove Henderson's results beginning with (2).

Suppose  $\begin{bmatrix} \tilde{\beta} \\ \tilde{u} \end{bmatrix}$  solves the MME.

Then

$$X'X\tilde{\beta} + X'Z\tilde{u} = X'y$$

and

$$Z'X\tilde{\beta} + (H^{-1} + Z'Z)\tilde{u} = Z'y.$$

The 2<sup>nd</sup> equation

$$\implies (\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})\tilde{\mathbf{u}} = \mathbf{Z}'\mathbf{y} - \mathbf{Z}'\mathbf{X}\tilde{\boldsymbol{\beta}}$$

$$\implies \tilde{\mathbf{u}} = (\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}})$$

$$\implies \tilde{\mathbf{u}} = \mathbf{HZ}'(\mathbf{I} + \mathbf{ZHZ}')^{-1}(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}}) \text{ by } (*)$$

$$\implies \tilde{\mathbf{u}} = \mathbf{HZ}'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}}) = \mathbf{GZ}'\boldsymbol{\Sigma}^{-1}(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}}).$$

Now this last expression for  $\tilde{u}$  indicates that  $\tilde{u}$  is the BLUP for  $u$  as long as  $\tilde{\beta}$  solves the Aitken equations.

To show this, we examine the 1<sup>st</sup> MME.

The 1<sup>st</sup> MME is

$$\mathbf{X}'\mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{X}'\mathbf{Z}\tilde{\mathbf{u}} = \mathbf{X}'\mathbf{y}.$$

We have shown

$$\tilde{\mathbf{u}} = (\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}}).$$

Combining these equations gives

$$\mathbf{X}'\mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{X}'\mathbf{Z}(\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}}) = \mathbf{X}'\mathbf{y}.$$

By Lemma H2,

$$\mathbf{Z}(\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}' = \mathbf{I} - \mathbf{V}^{-1}.$$

Thus,

$$\mathbf{X}'\mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{X}'(\mathbf{I} - \mathbf{V}^{-1})(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}}) = \mathbf{X}'\mathbf{y}$$

$$\iff \mathbf{X}'\mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{X}'\mathbf{y} - \mathbf{X}'\mathbf{X}\tilde{\boldsymbol{\beta}} - \mathbf{X}'\mathbf{V}^{-1}\mathbf{y} + \mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\tilde{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{y}$$

$$\iff \mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\tilde{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{V}^{-1}\mathbf{y}.$$

$\therefore \tilde{\boldsymbol{\beta}}$  solves the AE and Henderson's result (2) follows.

Now let's prove (3).

Suppose  $\tilde{\beta}$  solves the AE.

Let

$$\begin{aligned}\tilde{u} &= \mathbf{HZ}'\mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\tilde{\beta}) \\ &= \mathbf{HZ}'(\mathbf{I} + \mathbf{ZHZ}')^{-1}(\mathbf{y} - \mathbf{X}\tilde{\beta}) \\ &= (\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'(\mathbf{y} - \mathbf{X}\tilde{\beta}) \text{ by } (*)\end{aligned}$$

$$\implies (\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})\tilde{u} = \mathbf{Z}'(\mathbf{y} - \mathbf{X}\tilde{\beta}) = \mathbf{Z}'\mathbf{y} - \mathbf{Z}'\mathbf{X}\tilde{\beta}$$

$$\implies \mathbf{Z}'\mathbf{X}\tilde{\beta} + (\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})\tilde{u} = \mathbf{Z}'\mathbf{y}.$$



$\therefore 2^{nd}$  MME is satisfied.

Now

$$\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\tilde{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$$

$$\implies \mathbf{X}'[\mathbf{I} - \mathbf{Z}(\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})\mathbf{Z}']\mathbf{X}\tilde{\boldsymbol{\beta}} = \mathbf{X}'[\mathbf{I} - \mathbf{Z}(\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})\mathbf{Z}']\mathbf{y}$$

(By Lemma H2)

It follows that

$$\mathbf{X}'\mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{X}'\mathbf{Z}(\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}}) = \mathbf{X}'\mathbf{y}.$$

Now

$$\begin{aligned}\tilde{\mathbf{u}} &= (\mathbf{H}^{-1} + \mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'(\mathbf{y} - \mathbf{X}\tilde{\boldsymbol{\beta}}) \\ \implies \mathbf{X}'\mathbf{X}\tilde{\boldsymbol{\beta}} + \mathbf{X}'\mathbf{Z}\tilde{\mathbf{u}} &= \mathbf{X}'\mathbf{y}.\end{aligned}$$

$\therefore$  The 1<sup>st</sup> MME is satisfied and result (3) follows.

Result (1) is now easy to prove as follows.

The AE are consistent.

Thus, by Henderson's result (3), the MME are consistent. □

Now suppose  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u} + \mathbf{e}$ , where all is as before except that, instead of  $\text{Var}(\mathbf{e}) = \sigma_e^2 \mathbf{I}$ ,  $\text{Var}(\mathbf{e}) = \mathbf{R}$ , a symmetric, positive definite variance matrix.

Let  $\mathbf{S} = \frac{1}{\sigma_e^2} \mathbf{R}$ , where  $\sigma_e^2$  is a positive variance parameter.

Consider the transformation

$$\mathbf{S}^{-1/2} \mathbf{y} = \mathbf{S}^{-1/2} \mathbf{X} \boldsymbol{\beta} + \mathbf{S}^{-1/2} \mathbf{Z} \mathbf{u} + \mathbf{S}^{-1/2} \mathbf{e}.$$

Then  $\mathbf{S}^{-1/2}\mathbf{e} \sim N(\mathbf{0}, \sigma_e^2\mathbf{I})$ , and our previous results with

$\mathbf{S}^{-1/2}\mathbf{y}$ ,  $\mathbf{S}^{-1/2}\mathbf{X}$ , and  $\mathbf{S}^{-1/2}\mathbf{Z}$  in place of  $\mathbf{y}$ ,  $\mathbf{X}$ , and  $\mathbf{Z}$

yield the mixed model equations

$$\begin{bmatrix} \mathbf{X}'\mathbf{S}^{-1}\mathbf{X} & \mathbf{X}'\mathbf{S}^{-1}\mathbf{Z} \\ \mathbf{Z}'\mathbf{S}^{-1}\mathbf{X} & \mathbf{H}^{-1} + \mathbf{Z}'\mathbf{S}^{-1}\mathbf{Z} \end{bmatrix} \begin{bmatrix} \tilde{\boldsymbol{\beta}} \\ \tilde{\mathbf{u}} \end{bmatrix} = \begin{bmatrix} \mathbf{X}'\mathbf{S}^{-1}\mathbf{y} \\ \mathbf{Z}'\mathbf{S}^{-1}\mathbf{y} \end{bmatrix}.$$

Multiplying both sides by  $1/\sigma_e^2$  gives

$$\begin{bmatrix} X'R^{-1}X & X'R^{-1}Z \\ Z'R^{-1}X & G^{-1} + Z'R^{-1}Z \end{bmatrix} \begin{bmatrix} \tilde{\beta} \\ \tilde{u} \end{bmatrix} = \begin{bmatrix} X'R^{-1}y \\ Z'R^{-1}y \end{bmatrix}.$$

This is the more general form of Henderson's Mixed Model Equations.

Finally, let  $\hat{G}$  and  $\hat{R}$  denote  $G$  and  $R$  with unknown parameters replaced by their REML estimates.

In practice, we solve

$$\begin{bmatrix} X'\hat{R}^{-1}X & X'\hat{R}^{-1}Z \\ Z'\hat{R}^{-1}X & \hat{G}^{-1} + Z'\hat{R}^{-1}Z \end{bmatrix} \begin{bmatrix} \tilde{\beta} \\ \tilde{u} \end{bmatrix} = \begin{bmatrix} X'\hat{R}^{-1}y \\ Z'\hat{R}^{-1}y \end{bmatrix},$$

to get solutions needed for computation of BLUEs and BLUPs.